Architectural constraints required to attain 1 Exaflop/s for scientific applications

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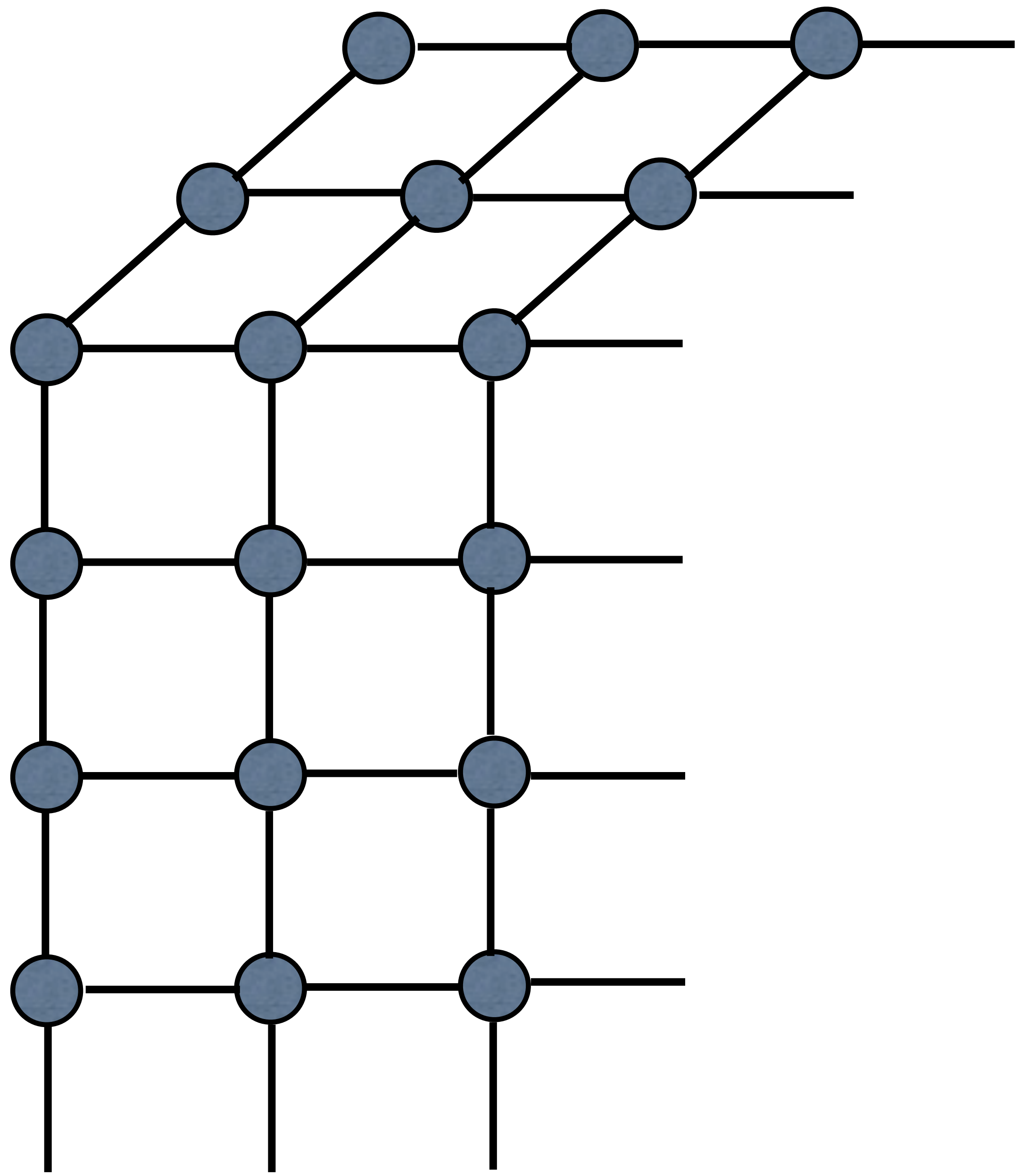
Motivation

- First Teraflop/s computer (ASCI Red, 1997), first Petaflop/s computer (RoadRunner, 2008), Exaflop/s 2018 ?
- Hardware challenges: power/energy, memory, communication
- Software challenges: algorithms and implementations that will scale
- Architectural features to attain 1 Exaflop/s ?

A possible exascale machine

- 2^{20} = 1,048,576 nodes
- 2^{10} cores per node
- 10 Gflop/s cores, time to compute a flop, t_c = 0.1 ns
- 10.74 Exaflop/s peak performance



Modeling methodology

- Estimate the floating point calculations/operations per iteration,

$$T_{comp} = \frac{1}{\eta} \times f(N, P_c) \times n \times t_c$$

- Time for communication based on number and size of messages

$$T_{comm} = M \times (t_s + h(N, P_c) \times t_w)$$

- Using total number of floating point operations and time per iteration, $\frac{flops}{T} > 10^{18}$

Applications

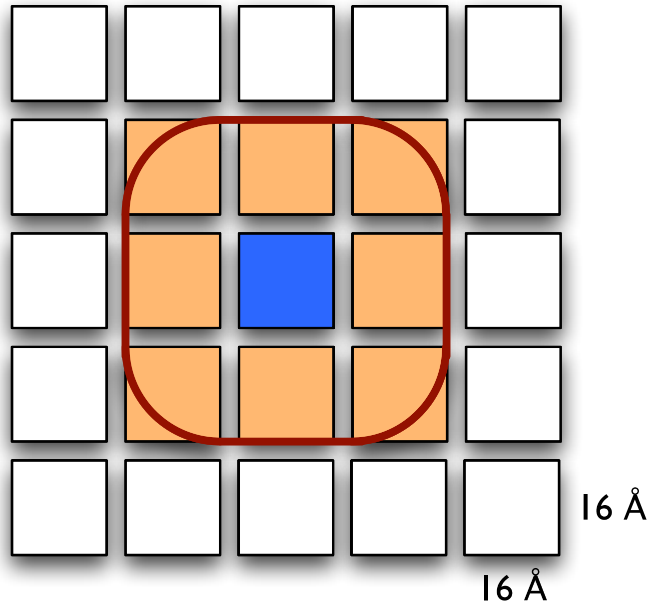
- Molecular Dynamics
  - Short-range forces, spatial decomposition
- Cosmological Simulations
  - Tree algorithms
- Unstructured grid problems
  - Finite element solvers

Molecular Dynamics

- Spatial decomposition

Algorithm 1 Computation in one time step of MD

```
Receive atoms from neighboring processors
for i = 1 to N_p do
    for j = 1 to N_i do
        if atoms are within cutoff radius, r_c then
            Compute forces on pairs of atoms
        end if
    end for
end for
Update atom positions and velocities
```



Weak scaling of MD

- Size of molecular system = 100 * 2^{30} = 107 billion atoms
- Number of floating point operations = 33547 * N

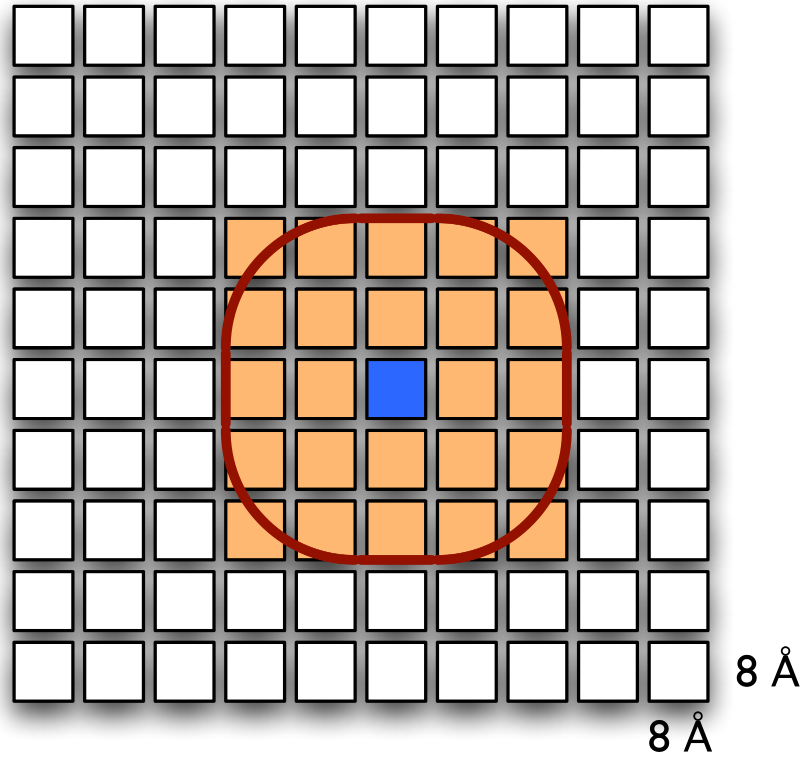
$$\frac{flops}{T} > 10^{18}$$

$$\frac{33547 \times N}{10^{18}} > T$$

- Putting N = 100 * 2^{30},

$$T < 3.6 \times 10^{-3}$$

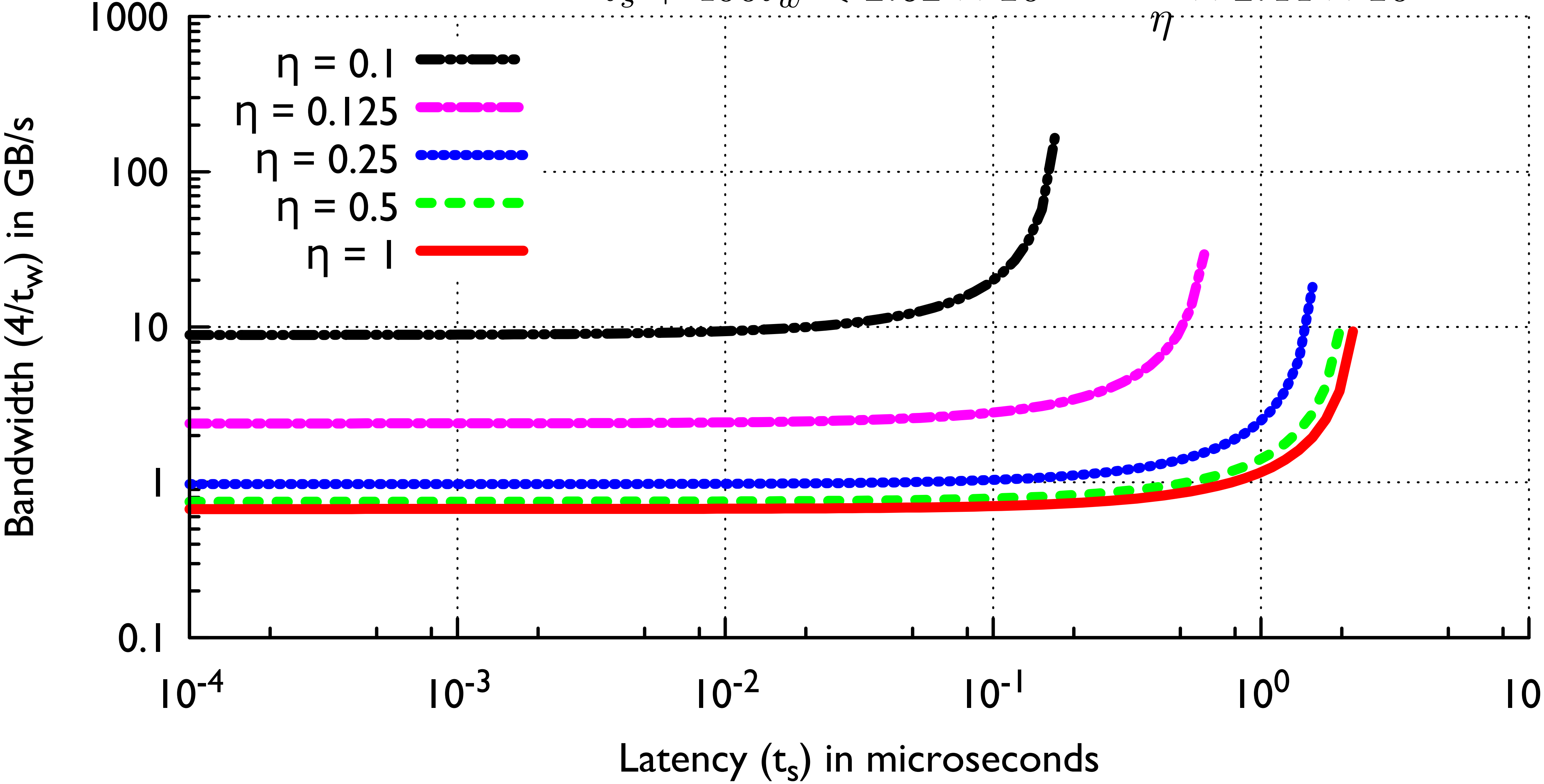
- 100 atoms per cell
- Split the cells in two of the three dimensions
- Each cell communicates with 5*5*3 = 75 other cells
- For a block of 8*8*16 cells placed on a node only the ones on the boundary communicate inter-node



Inferring network parameters

$$\frac{1}{\eta} \times \frac{N}{P_c} \times 33547 \times t_c + 1376 \times \left(t_s + \frac{N}{P_c} 4t_w\right) < 3.6 \times 10^{-3}$$

$$t_s + 400t_w < 2.62 \times 10^{-6} - \frac{1}{\eta} \times 2.44 \times 10^{-7}$$



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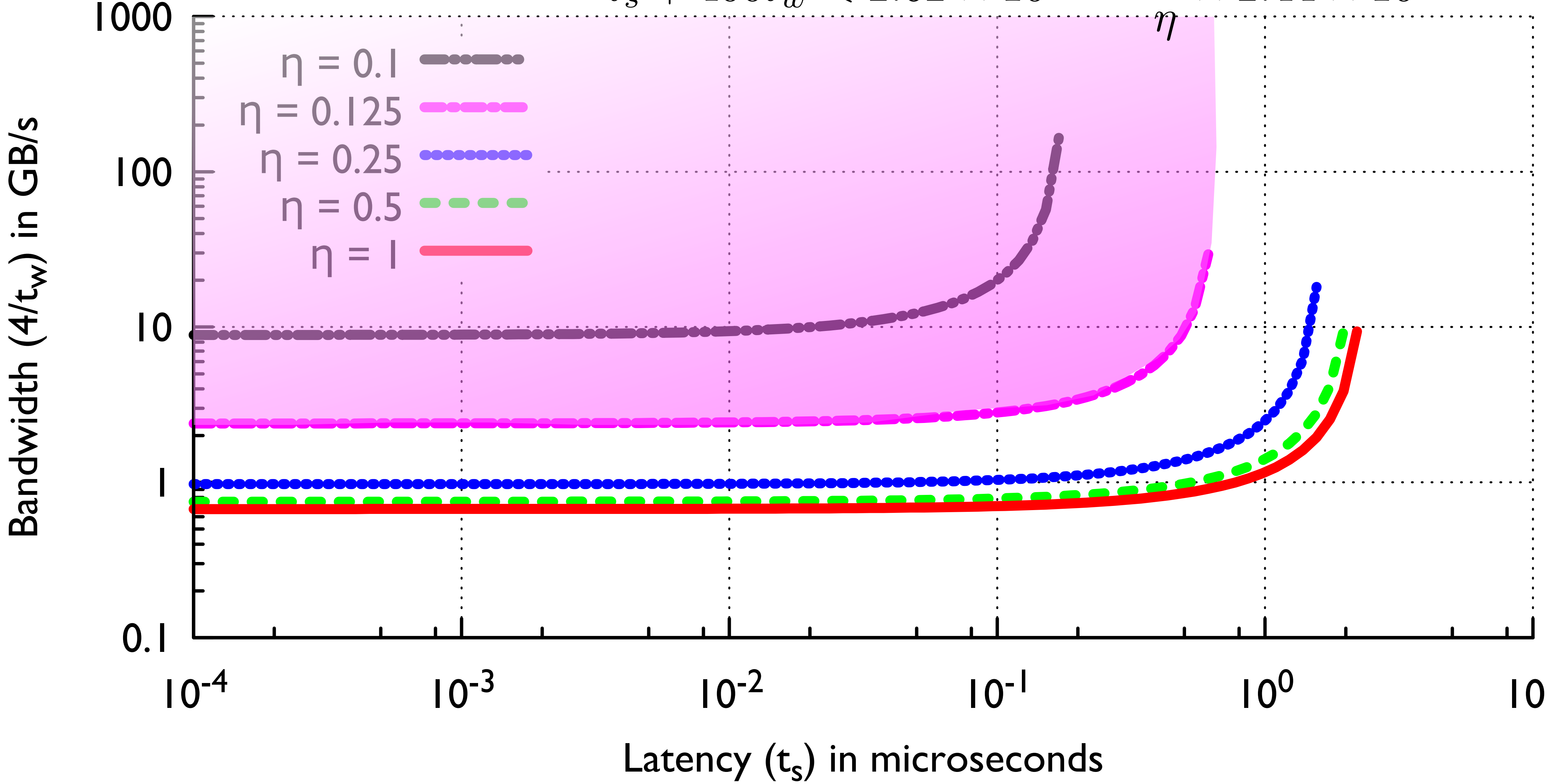
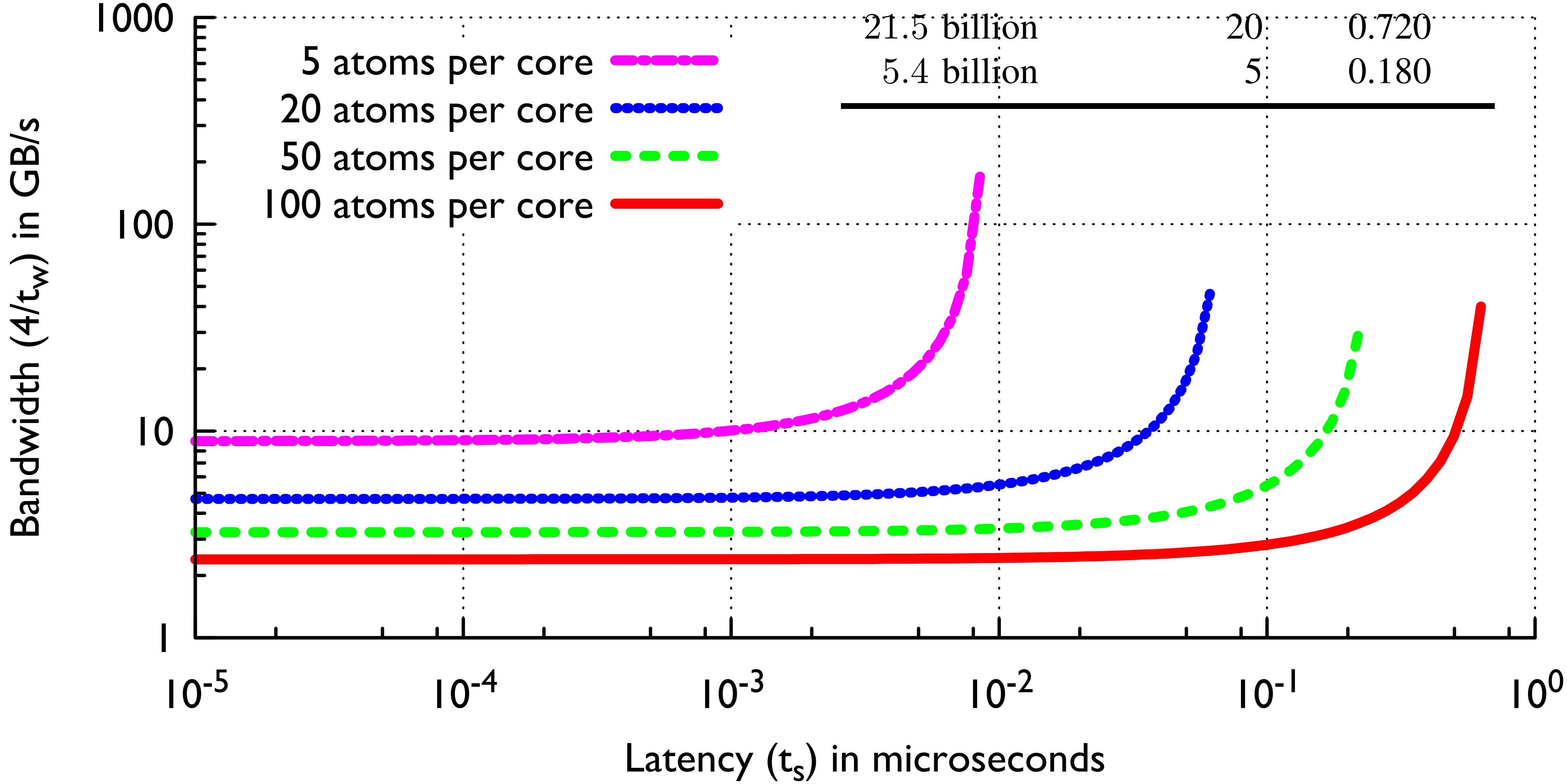


Smaller problem sizes

# Atoms	Atoms/core	Time (ms)
107 billion	100	3.602
53.6 billion	50	1.801
21.5 billion	20	0.720
5.4 billion	5	0.180



Computational Cosmology

- Several approaches to computing trajectories of bodies under gravitational attraction
  - Direct, all-pairs
  - Tree-based approximate methods
  - Particle-mesh or "grid" methods
- We consider locality-aware tree codes

Modeling problem size

- What problems will be of interest given an exascale-level machine
- Extrapolate from current state-of-the-art simulations
- About 8192 particles are required per core for good parallel efficiency at petascale
- Given O(N log N)/P work per core, about 6350 particles per core are needed at exascale (total 6.8 trillion)

Barnes-Hut computation

- Analyze algorithm:
  - Domain decomposition => distributed spatial tree
  - Every processor core gets a number of leaves
  - For each leaf l, Traverse(l, root)

```
Traverse(leaf l, node n) {
  if(IsLeaf(n)) {
    LeafForces(l, n);
  }
  else if(Side(n)/|r(n)-r(l)| < Θt)
{
    CellForces(l, n);
  }
  else {
    foreach(node c in Children(n)) {
       Traverse(l, c);
  }
}
```

Total computation

- Number of floating point operations per iteration,

$$312 \times 77 \times N \times \lg \frac{N}{B} + 38 \times 33 \times B \times N$$

- To attain a rate of 1 Exaflop/s,

$$\frac{24024 \times N \lg(N/B) + 1254 \times BN}{T} > 10^{18}$$

- T < 6.52s

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- However, cores on an SMP node can reuse remote data through software caching
- Communication with remote data caching:
  - Each SMP node holds a cube of space
  - Cores holding particles near surface of cube request remote data - other cores reuse data
  - Find each SMP node's *halo* of requests at each level of tree

Communication analysis

Leaf level:

$12n_b^2 + 36n_b + 8$

1 level above leaves:

$12(n_b/2)^2 + 36(n_b/2) + 8$

2 levels above leaves:

$12(n_b/4)^2 + 36(n_b/4) + 8$

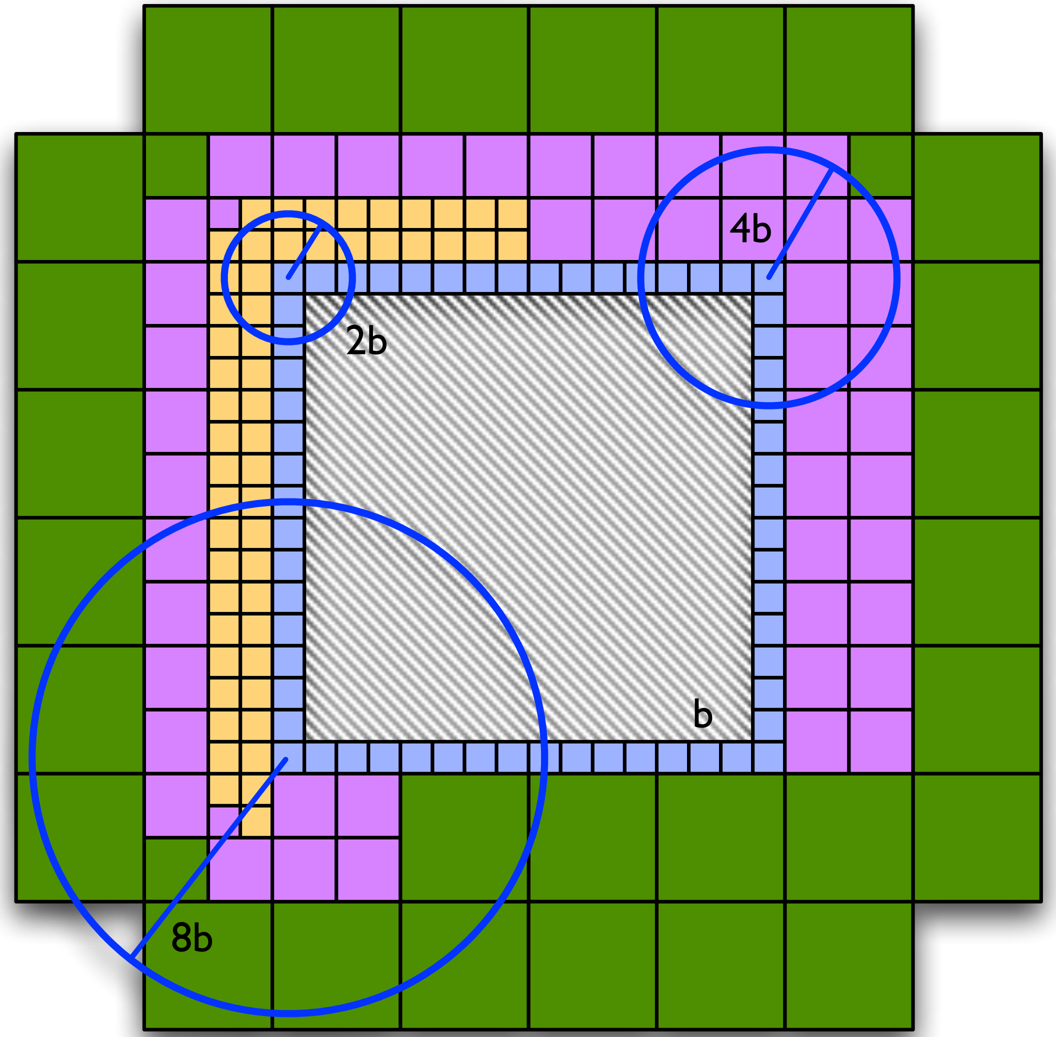
3 levels above leaves:

$12(n_b/8)^2 + 36(n_b/8) + 8$

...

Total:

$$C_1^{\text{cell}} = \sum_{i=0}^{\lg n_b} \left(12 \left(\frac{n_b}{2^i} \right)^2 + 36 \left(\frac{n_b}{2^i} \right) + 8 \right)$$
$$= 16n_b^2 + 72n_b + 8 \lg n_b - 32 \quad \text{cells}$$



Upper-level calls

- Previous reasoning valid as long as edge length of requested calls <= $c/(P_n)^{1/3}$
- Use reasoning similar to calculation of E(l) to get number of larger, upper-level cells requested per SMP node,

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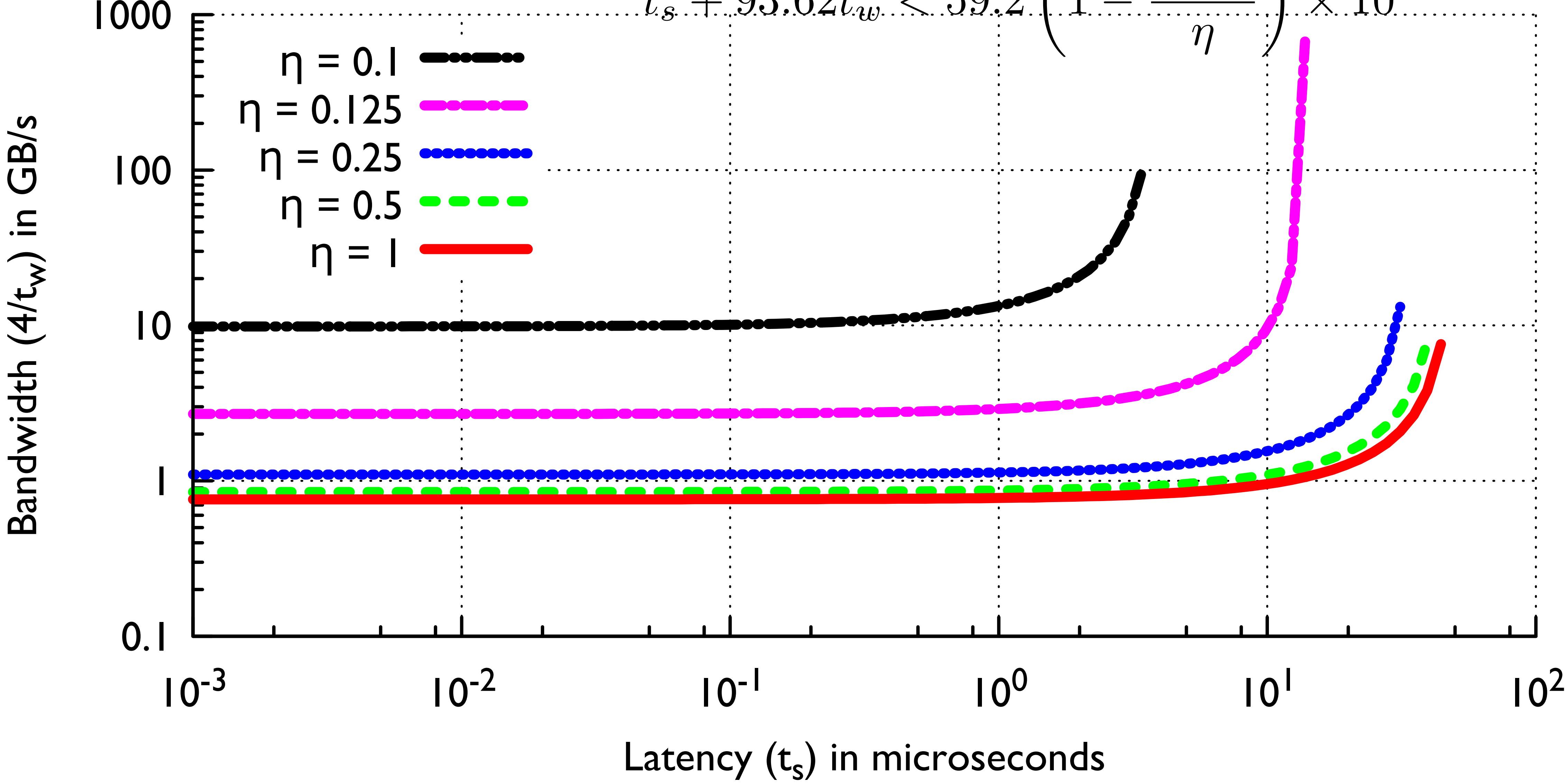
$$C_2^{\text{cell}} = 31\left(\frac{\lg P_n}{3} - 1\right) \quad \text{cells}$$

$$T_{comm} = 15946(t_s + 56t_w) + 93968(t_s + 100t_w)$$

Inferring network parameters

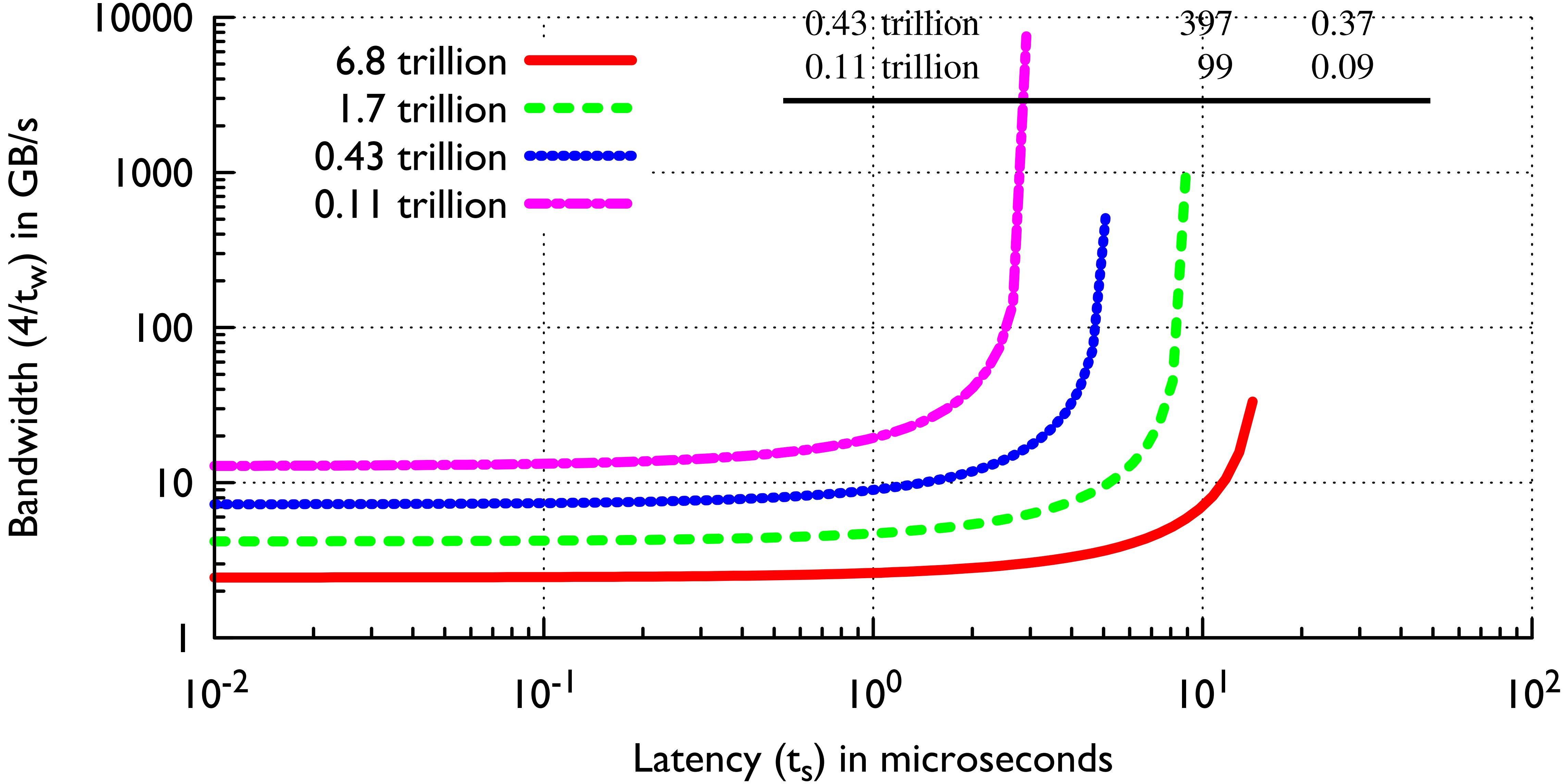
$$\frac{6.52 \times 10^{18}}{P_c} \times \frac{t_c}{\eta} + (1.1 \times 10^5 t_s + 1.03 \times 10^7 t_w) < 6.52$$

$$t_s + 93.62 t_w < 59.2 \left(1 - \frac{0.093}{\eta}\right) \times 10^{-6}$$



Smaller problem sizes

# Particles	Particles/core	Time (s)
6.8 trillion	6350	6.52
1.7 trillion	1588	1.55
0.43 trillion	397	0.37
0.11 trillion	99	0.09

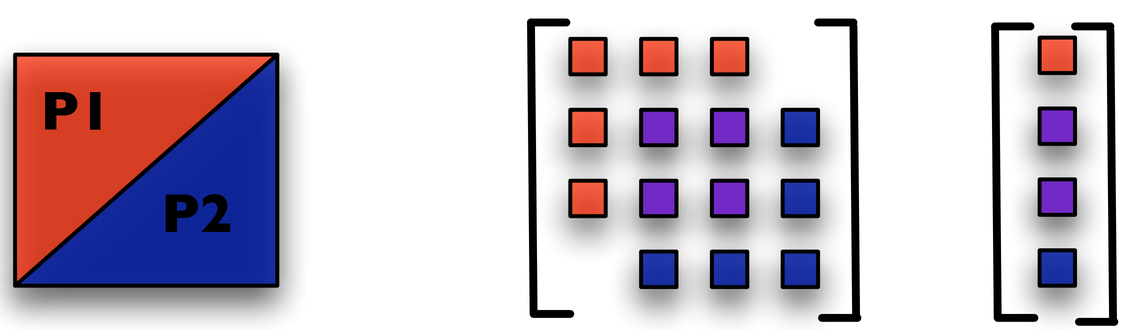


Finite Element Solvers

- Method of choice for unstructured grid problems
- Involves two phases:
  - Assembly: put linear system together
  - Solve: the system
- Linear problems: one assembly, one (time-independent) or more (time-dependent) solves
- Nonlinear problems: repeat assembly/solve process until convergence

Approach to Solution

- Based on recent work by Sahni et al. that scales FEM to near-petascale
- Partition the problem by elements, storing shared DOFs redundantly



- Assembly becomes nearest-neighbor: focus on solve

Approach to Solution

- Assume conjugate gradient linear solver
  - Setup: one mat-vec product, one vector subtraction, one dot product
  - Iteration loop: one mat-vec product, two vector additions, one vector subtraction, two dot products

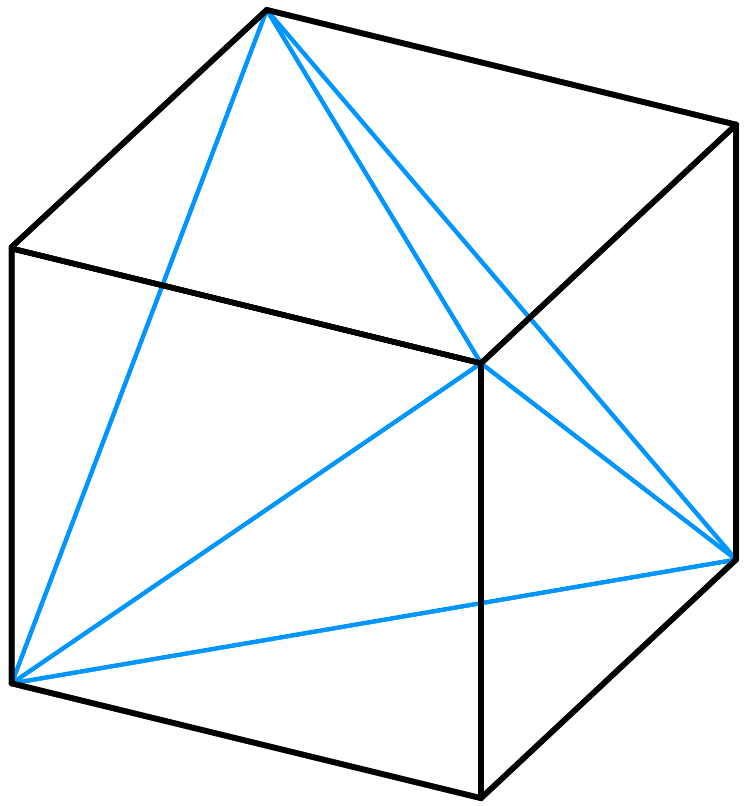
Algorithm 3 CG(A,b,x_0,$rtol$)

$r_0 \leftarrow b - Ax_0$
$p_0 \leftarrow r_0$
$k \leftarrow 0$
while $||r_k||_2 \geq rtol$ **do**
  $\alpha_k \leftarrow \frac{r_k^T r_k}{p_k^T A p_k}$
  $x_{k+1} \leftarrow x_k + \alpha_k p_k$
  $r_{k+1} \leftarrow r_k - \alpha_k A p_k$
  $\beta_k \leftarrow \frac{r_{k+1}^T r_{k+1}}{r_k^T r_k}$
  $p_{k+1} \leftarrow r_{k+1} + \beta_k p_k$
  $k \leftarrow k + 1$
end while
return x_k

FEM: Weak Scaling

- Consider problem on 3D cubic tet mesh
  - Each core gets 16^3 cubes
  - Degrees of freedom on each processor = 17^3
- Global DOFs = 4.4 trillion
- Solve time per iteration:

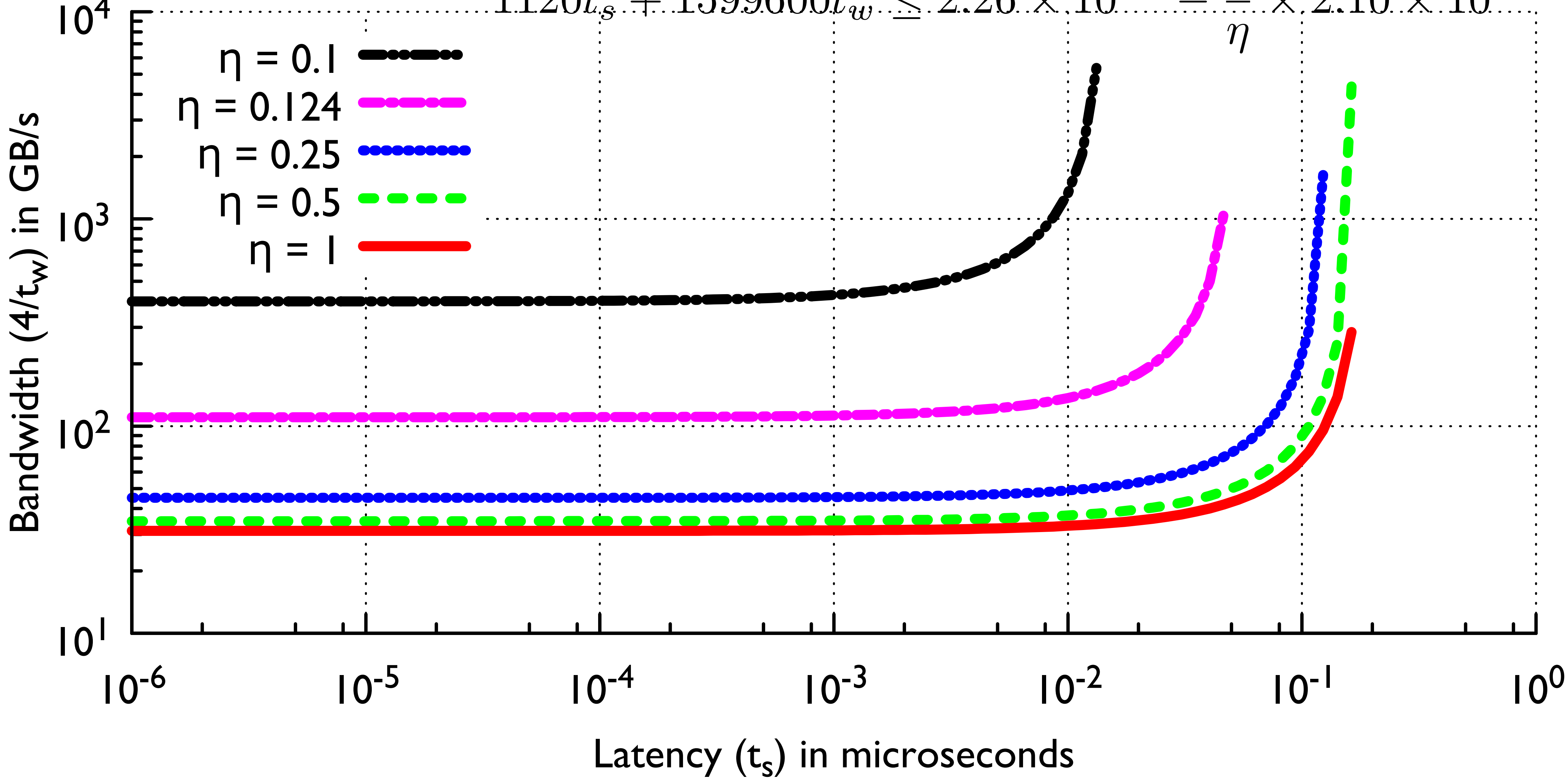
$$T_{\text{CG}}^{\text{iter}} = \frac{1}{\eta} \times \left((2s_i + 6)n_i + \frac{N}{P_c} + 2\lg P_n \right) t_c \\ + 2(520 + 2\lg P_n)t_s \\ + 2(520\tilde{n}_i + 2\lg P_n)t_w$$



Inferring network parameters

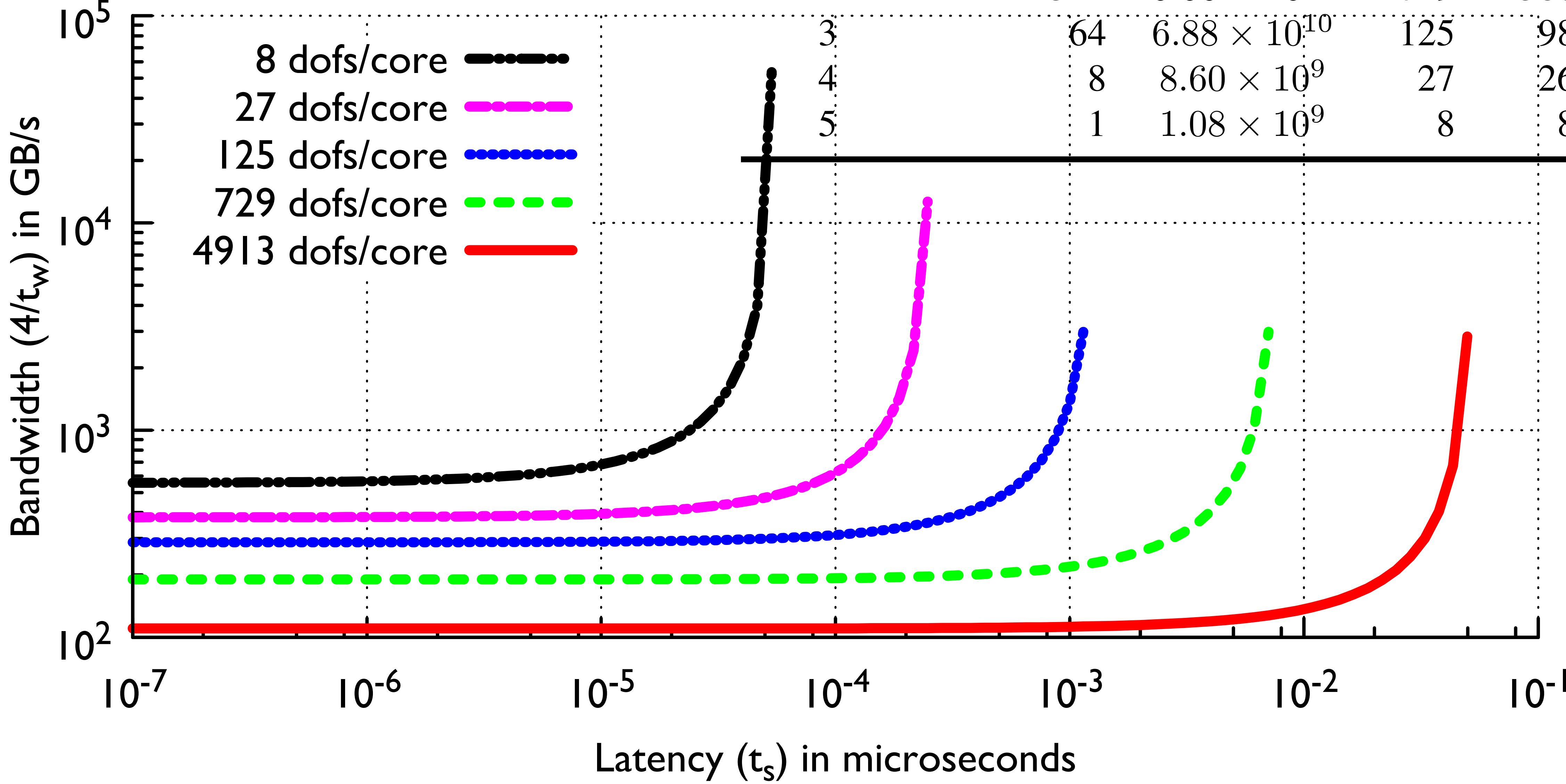
$$\frac{P_c(2s_i+1)n_i + N + 2\lg P_n}{T_{\mathrm{CG}}^{\mathrm{iter}}} \geq 10^{18}$$

$$1120t_s + 1599600t_w \leq 2.26\times10^{-4} - \frac{1}{\eta}\times 2.10\times10^{-5}$$



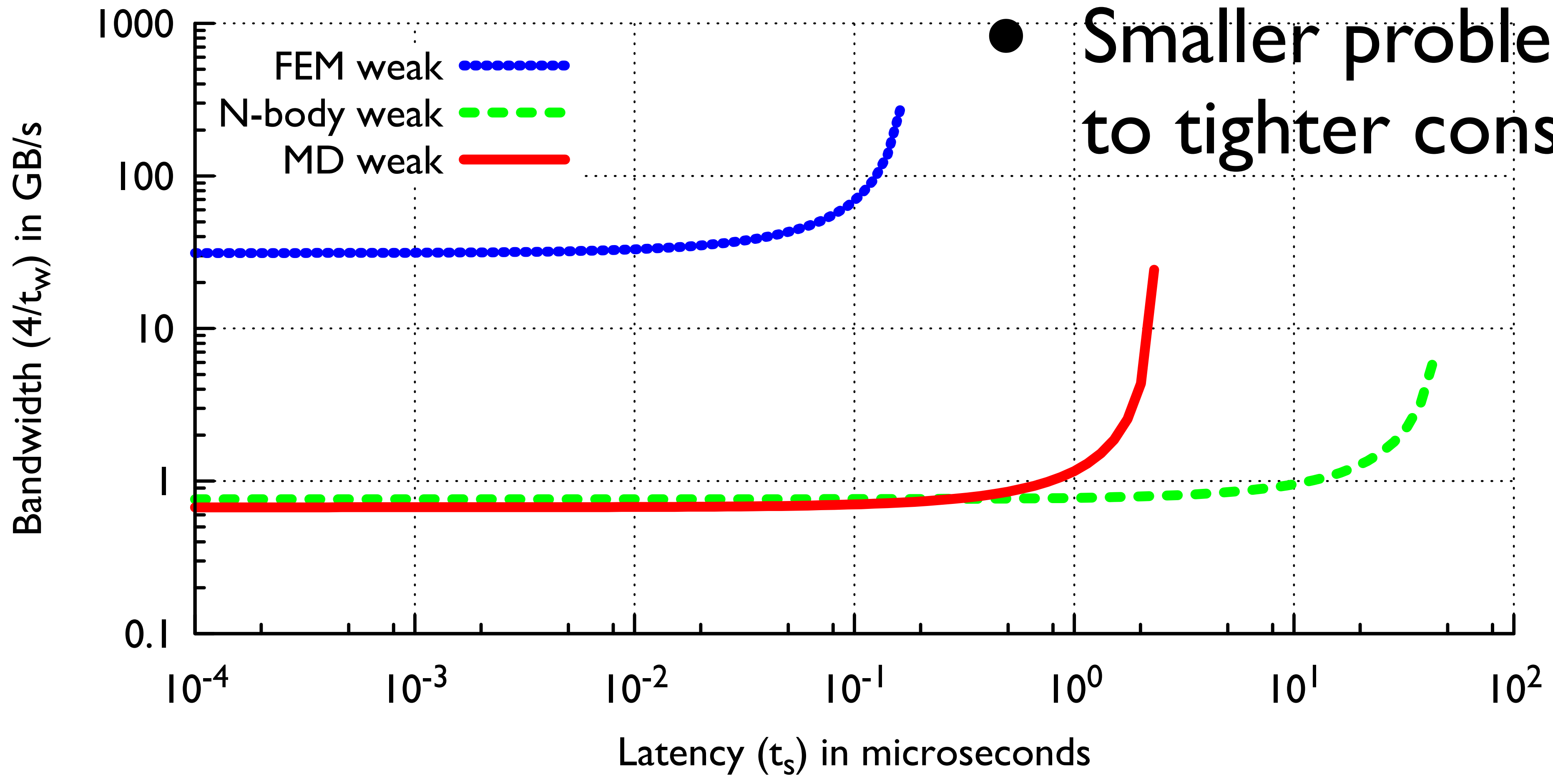
Smaller problem sizes

Problem	Cubes/core	N	n_i	$\tilde{n}_i$
1	4096	4.40×10^{12}	4913	1538
2	512	5.50×10^{11}	729	386
3	64	6.88×10^{10}	125	98
4	8	8.60×10^{9}	27	26
5	1	1.08×10^{9}	8	8



Summary

- Modest communication requirements for MD and cosmology at exascale
- Smaller problem sizes lead to tighter constraints



Future work

- Research required in area of communication-minimizing algorithms and high-bandwidth low-latency networks
- Detailed analysis of each application class
  - MD: long-range forces
  - Cosmology: particle-mesh methods
  - FEM: other solvers, preconditioning
- Studies for specific networks and contention